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Workshop on Understanding Quantum Phenomena with Path Integrals: From Chemical Systems to Quantum fluids and Solids | (smr 3131)

Wednesday 05 July 2017

Morning Chairmen: Ondrej MARSALEK & Marco NAVA / Afternoon Chairmen: Nancy MAKRI & Sebastiano PILATI - Kastler Lecture Hall (AGH) (09:00-21:00)

time	title	presenter
09:00	Hydrogen Diffusion and Lithium Isotope Fractionation: Cases of Competing and (sometimes) Surprising Quantum Effects	TUCKERMAN, Mark
09:50	Path Integral Methods for Nonadiabatic Dynamics: Quantum Transitions from Classical Trajectories	ANANTH, Nandini
10:40	Coffee break	
11:10	Rigorous Quantum-Classical Path Integral Formulation of Real-Time Dynamics	MAKRI, Nancy
12:00	High Order Path Integrals Made Easy	KAPIL, Venkat
12:20	Lunch break	
14:15	An Electronically Coarse Grained Model describes Water's Properties from Ice to the Supercritical Regime	MARTYNA, Glenn J.
15:05	Quantum Transport of Ions through Atomically Thin Materials	POLTAVSKYI, Igor
15:55	Coffee break	
16:25	Hanbury Brown-- Twis Effect in Finite-Sized Bose Gases	SCHUMAYER, Daniel
16:45	Flash Talks Session	
	- 16:45 - Superfluidity in a System of Polarized Dipolar Bosons	BOMBIN ESCUDERO, Raul
	- 16:49 - Analysis and Benchmark of Non-Adiabatic Dynamics with NRPMD	CALDERINI, Danilo
	- 16:53 - Thermal Field Theory of Bosonic Gases with Finite-Range Effective Interaction	CAPPELLARO, Alberto
	- 16:57 - A Semiclassical Divide-and-Conquer Method for Spectroscopic Calculations of High Dimensional Molecular Systems	DI LIBERTO, Giovanni
	- 17:01 - Quantum and Thermal Effects in the Melting of Simple Solids	DUSSEAUULT, Marisa
	- 17:05 - Hydrogen Atom Abstraction from Ethanol by Atomic Hydrogen in Aqueous Solution	KANNATH, Suraj
	- 17:09 - Inclusion of Quantum Nuclear Effects in Alkanes using PIMD Techniques	KONDRATYUK, Nikolay
	- 17:13 - Nuclear Quantum Effects on Surface-Assisted Water Dissociation	LITMAN, Yair
	- 17:17 - Spin Dynamics in One-Dimensional Bosonic Quantum Gases	PARISI, Luca
	- 17:21 - Nuclear Quantum Effects on Acid Dissociation in Microsolvation Environments	PEREZ DE TUDELA, Ricardo
	- 17:25 - Nuclear Quantum Effects in an HIV/Cancer Inhibitor: The Case of Ellipticine	SAPPATI, Subrahmanyam

	- 17:29 - From Quantum Fluids to Emergent Gravity: Quantum Potential Induced Non-Local BEC & Analogue Hawking Radiation	SARKAR, Supratik
	- 17:33 - Negativity of Wigner Function as Measure of Quantum Correlations	SIYOURI, Fatima-Zahra
	- 17:37 - Signatures of Inequivalent Representations in Path Integrals	SMALDONE, Luca
	- 17:41 - Efficient Simulation of Non-Markovian Open Systems using Real Time Path Integrals	STRATHEARN, Aidan
	- 17:45 - Path Integral Methods to Compute Electron Transfer Reaction Rates	THAPA, Manish
	- 17:49 - Relaxation Dynamics in Isolated and Open Many-Body Quantum Systems	URANGA PINA, Llinersy
	- 17:53 - Microcanonical Instanton Rate Theory Applied to Molecular Reactions	WINTER, Pierre
	- 17:57 - Nuclear Quantum Effects and Isotope Effects for Vaporation of Dibromomethane	VASQUEZ, Luis
	- 18:01 - Thermodynamics of the Unitary Bose Gas from First Principles	COMPARIN, Tommaso
	- 18:05 - Adsorption of Molecular Hydrogen on Nanostructured Surfaces	MARTINEZ MESA, Aliezer
18:15	Poster Session with Refreshments (outside the Kastler Lecture Hall, lower level)	